C:\Program Files\STNEXP\Queries\10590458.str

chain nodes : 18 19 20 21 22 23 24 25 ring nodes : 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 chain bonds : 1-15 4-18 4-19 6-20 6-21 7-22 23-25 24-25

ring bonds :

1-2 1-7 2-3 2-8 3-4 3-11 4-5 5-6 6-7 8-9 9-10 10-11 12-13 12-17 13-14 14-15 15-16 16-17 exact/norm bonds : 1-2 1-7 3-4 4-5 4-18 4-19 5-6 6-7 7-22 23-25 24-25

exact bonds :

1-15 6-20 6-21 normalized bonds :

2-3 2-8 3-11 8-9 9-10 10-11 12-13 12-17 13-14 14-15 15-16 16-17

Match level : 1.1 level ; 1.1 level ; 2.1 le